Localization properties of a one-dimensional tight-binding model with non-random long-range inter-site interactions

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We perform both analytical and numerical studies of the one-dimensional tight-binding Hamiltonian with stochastic uncorrelated on-site energies and non-fluctuating long-range hopping integrals $J_{mn} = J/|m-n|^{\mu}$. It was argued recently [A. Rodríguez *at al.*, J. Phys. A: Math. Gen. **33**, L161 (2000)] that this model reveals a localization-delocalization transition with respect to the disorder magnitude provided $1 < \mu < 3/2$. The transition occurs at one of the band edges (the upper one for $J > 0$ and the lower one for $J < 0$). The states at the other band edge are always localized, which hints on the existence of a single mobility edge. We analyze the mobility edge and show that, although the number of delocalized states tends to infinity, they form a set of null measure in the thermodynamic limit, i.e. the mobility edge tends to the band edge. The critical magnitude of disorder for the band edge states is computed versus the interaction exponent μ by making use of the conjecture on the universality of the normalized participation number distribution at transition.

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I. INTRODUCTION

In 1958 Anderson formulated a simple tight-binding model with uncorrelated on-site (diagonal) disorder and predicted a localization-delocalization transition (LDT) in three dimensions (3D): a phase of extended states appears at the band center in the thermodynamic limit if the disorder magnitude is smaller than a critical value, while all states are localized at larger magnitudes of disorder.[1] The phase of delocalized states is separated from the two phases of localized states by two mobility edges.[2] The concept of the mobility edge is of key importance for the low-temperature transport properties of disordered materials.

Since the advent of the single-parameter scaling hypothesis, introduced by Abrahams *et al.*,[3] the occurrence of a localization-delocalization transition (LDT) in disordered systems with time reversal symmetry was ruled out in one- (1D) and two dimensional (2D) geometries at any disorder strength (for the overview see Refs. 4,5,6,7). The localized nature of the states in 1D was pointed out even earlier by Mott and Twose.[8]

At the end of eighties and beginning of nineties it was realized however that correlations in disorder may give rise to extended states in low dimensions.[9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24] Thus, short-range correlated on-site disorder was found to cause the appearance of extended states at special resonance energies in 1D. They form a set of null measure in the density of states in the thermodynamic limit,[9,10,11,12,13,14] implying the absence of the mobility edges in those models. In spite of this fact, even the infinitesimal fraction of the extended states may have a strong impact on the transport properties of disordered materials. In particular, short-range correlations in disordered potential were put forward to explain unusual conducting properties of polymers, such as polyaniline and heavily doped polyacetylene,[11,12] as well as semiconductor superlattices grown with random but correlated quantum well sequences.[15]

Contrary to short-range correlations in the disorder distribution, long-range correlations were demonstrated to cause the LDT in 1D systems, which is analogous to the standard Anderson LDT in 3D.[16,17,18,19,20,21] In this regard, a 1D system with nearest-neighbor interactions and long-range correlated on-site disorder distribution with a power-like spectrum $S(k) \sim k^{-\alpha}$ is critical with respect to the exponent α. More specifically, when the standard deviation of the energy distribution equals the nearest-neighbor hopping and $\alpha < 2$ all states are localized, while for $\alpha > 2$ a phase of extended states appears at the center of the band giving rise to two mobility edges. The phase occupies a finite fraction of the density of states. A similar picture holds in 2D.[23] The authors of Ref. 18 proposed to use the long-range correlated disorder and the appearance of a phase of extended states for designing microwave filters based on a single-mode waveguide. This type of disorder is also being studied in biophysics in connection with the large-distance charge transport in DNA sequences.[25,26]

Another 1D model which exhibits the LDT and a phase of extended states is an ensemble of power-law random banded matrices $H_{ik} \propto G_{ik}\,|i-k|^{-\alpha}$, where the matrix G_{ik} runs over a Gaussian orthogonal ensemble[27,28] (for an overview see Ref. 29). This model is critical *with respect to the interaction exponent* α: for $\alpha > 1$ all states are localized, while all of them are delocalized at $\alpha < 1$, suggesting that $\alpha = 1$ is the critical point in the model. Within the framework of this model, it was demonstrated rigorously that (i) the distribution function of the inverse participation ratio is scale invariant at transition and

(ii) the relative fluctuation of the inverse participation ratio (the ratio of the standard deviation to the mean) is of the order of unity at the critical point.[30,31] This finding confirmed the conjecture (which was put forward earlier[32,33]), that distributions of relevant physical magnitudes are universal at criticality (see also Refs. 34,35,36). The invariance can therefore be used to monitor the critical point.[37,38]

Recently, several reports addressed to the unusual localization properties of 1D and 2D tight-binding models with uncorrelated diagonal disorder and *non-random* long-range coupling between sites $\mathbf{m}$ and $\mathbf{n}$, which falls according to a power law $J/|\mathbf{m}-\mathbf{n}|^{\mu}$,[37,38,39,40,41,42] (see also Refs. 43-44). More specifically, the states at one of the band edges (the upper one for $J>0$ and the lower one for $J<0$) undergo the LDT *with respect to the disorder strength* Δ if the interaction exponent μ ranges within the interval $1<\mu<3d/2$, d being the dimensionality.[41] In what follows we set $J>0$, so that extended states can appear at the upper band-edge. The states at the other band-edge are strongly localized, no matter how small the disorder magnitude is, thus, suggesting the existence of a single mobility edge.[40] At $\mu \geq 3d/2$ all states were found to be localized. The character of localization, however, turned out to be governed by the interaction exponent μ. At $\mu = 3d/2$, the upper band-edge states are weakly localized, similar to those at the center of the band in the standard 2D Anderson model,[3] while at $\mu > 3d/2$ they are strongly localized.

In the present paper we deal with the analysis, both numerical and analytical, of the localization properties of the latter class of 1D Hamiltonians. We calculate the phase diagram of the transition for the upper band-edge states, i.e., the critical disorder magnitude Δ_c versus the interaction exponent μ, and show that Δ_c vanishes as $(3/2-\mu)^{2/3}$ when $\mu \to 3/2$, while it diverges as $(\mu-1)^{-1}$ when $\mu \to 1$. Applying the finite size scaling analysis we study the problem of the mobility edge and show that the mobility edge approaches to the upper band edge in the thermodynamic limit. In other words, the fraction of the delocalized states forms a set of null measure, although their number tends to infinity on increasing the system size N as $N^{(3/2-\mu)/(2-\mu)}$ (note that the dependence is sub-linear). This numerical finding is supported by a simple qualitative arguments based on the comparison of size scaling of two magnitudes: the bare level spacing at the band-edge and effective disorder *seen* by the quasiparticle.

The outline of the paper is as follows. In the next Section, we describe the model and briefly overview qualitative arguments which brought us to the conjecture on the existence of the LDT within the model. In Sec. III, we present the phase diagram of the LDT for the upper band-edge states, which is calculated on the basis of the statistics of the participation number. The mobility edge and fraction of the delocalized states are addressed in Sec. IV. We conclude the paper in Section V.

II. MODEL AND QUALITATIVE REASONING

We consider a tight-binding Hamiltonian on a 1D *regular* lattice with N sites

$$\mathcal{H} = \sum_n \varepsilon_n |n\rangle\langle n| + \sum_{nm} J_{mn} |m\rangle\langle n| \ . \qquad (1)$$

Here $|n\rangle$ is the ket vector of a state with on-site energy ε_n. These energies are taken at random and uncorrelated for different sites and distributed uniformly around zero within the interval $[-\Delta/2, \Delta/2]$, having therefore zero mean, $\langle \varepsilon_n \rangle = 0$, and standard deviation $\langle \varepsilon_n^2 \rangle^{1/2} = \Delta/\sqrt{12}$ (the angle brackets $\langle \cdots \rangle$ denote average over disorder realizations). The hopping integrals J_{mn} do not fluctuate and are set in the form $J_{mn} = J/|m-n|^{\mu}$, with $J>0$ and $J_{nn}=0$.

First, we address the disorder-free system ($\Delta = 0$), taking periodic boundary conditions for the sake of simplicity. Then the eigenstates of the Hamiltonian (1) are plane waves with quasi-momenta $K = 2\pi k/N$ within the first Brillouin zone $k \in [-N/2, N/2)$. The corresponding eigenenergies are given by

$$E_{\mu}(K) = 2J \sum_{n>0} \frac{\cos(Kn)}{|n|^{\mu}} \ , \qquad (2)$$

where the summation runs over all N sites of the lattice, and μ is assumed to be larger than unity to get a bounded energy spectrum. The complete account for all terms in the sum (2) is important in the neighborhood of the upper band-edge, where the long-range hopping terms affect the dispersion vastly. At the upper band-edge ($K \to 0$) the dispersion relation (2) is as follows[42]

$$E_{\mu}^{\rm top}(K) = E_{\rm top}(\mu) - J\, A_{\rm top}(\mu) |K|^{\mu-1} - J\, B_{\rm top}(\mu) K^2 \ , \qquad (3)$$

when $\mu \neq 3$. Here, $E_{\rm top}(\mu) = 2J \sum_n^{\infty} n^{-\mu} = 2J\zeta(\mu)$ is the upper band-edge energy in the thermodynamic limit, $A_{\rm top}(\mu)$ and $B_{\rm top}(\mu)$ are dimensionless positive constants on the order of unity (for brevity we do not provide explicit expressions for them), and $\zeta(\mu)$ is the Riemann ζ-function. For small K, the sub-quadratic term in the right-hand side of Eq. (3) dominates over the quadratic one if $\mu < 3$ and *vice versa*. The range $\mu < 3$ will be of our primary interest. We will focus later on the size scaling of the energy spacing at the upper band edge at $\mu < 3$, which is

$$\delta E_{\mu}^{\rm top} \propto N^{1-\mu} \ . \qquad (4)$$

At the lower band edge ($|K| \to \pi$), the energy spectrum is parabolic:

$$E_{\mu}^{\rm bot}(K) = E_{\rm bot}(\mu) + J\, B_{\rm bot}(\mu)\, (\pi - K)^2 \ , \qquad (5)$$

where $E_{\rm bot}(\mu) = 2\, J \sum_n^{\infty} (-1)^n n^{-\mu}$ is the lower band energy, which depends weakly on μ, and $B_{\rm bot}(\mu)$ is a dimensionless constant on the order of unity. Respectively,

the energy spacing at the bottom of the band scales as

$$\delta E_\mu^{\rm bot} \propto N^{-2} \ . \tag{6}$$

On introducing the disorder the eigenstates of the regular system couple to each other, which can result in their localization. The typical fluctuation of the coupling matrix, namely the first term on the right-hand side of Eq. (1) in the K-space basis, is[40]

$$\sigma = \frac{\Delta}{\sqrt{12N}} \ . \tag{7}$$

Now, we compare the size dependence of σ to that of the eigenenergy spacing at the top of the band $\delta E_\mu^{\rm top}$ (defined by Eq. (4)). As the system size increases the typical value of the eigenstate coupling σ decreases faster than the energy spacing $\delta E_\mu^{\rm top}$ at $\mu < 3/2$. Consider a system of size N and let σ be of *perturbative* magnitude (i.e. $\sigma \ll \delta E$), then the upper band-edge states are only weakly perturbed by disorder and remain extended over the whole system. Upon increasing the system size, the inequality $\sigma \ll \delta E$ gets even stronger, so that the perturbation becomes weaker and therefore the upper states will remain delocalized at $N \to \infty$. On the other hand, large disorder (say, larger than the bare bandwidth) would certainly localize all the states. These arguments indicate that there can exist extended states at the upper band-edge at finite disorder, provided that $1 < \mu < 3/2$. This conjecture was confirmed both theoretically, by means of the renormalization group approach combined with a super-symmetric method for disorder averaging[41], and numerically.[37,38,40] The value $\mu = 3/2$ represents the marginal case in which the upper band-edge states are localized weakly.[37,38,41] In what follows, we focus therefore on the interaction exponent μ ranging within the interval $1 < \mu \leq 3/2$.

At the bottom of the band ($|K| \to \pi$) the level spacing diminishes as N^{-2}, that is faster than the effective magnitude of disorder σ. Thus, even if $\sigma \ll \delta E$ for some lattice size and the states are extended over the whole system, the inequality will be reversed for larger N, which will finally result in strong coupling of the states and their eventual localization. The same conclusion holds for the entire energy spectrum if $\mu > 3/2$.

The above picture implies the existence of a single mobility edge separating the phases of localized and delocalized states. We address this question in detail in Sec. IV.

III. PHASE DIAGRAM OF THE TRANSITION

In this Section we calculate the dependence of critical disorder magnitude Δ_c on the interaction exponent $\mu \in (1, 3/2]$. To detect the transition we analyze the wave function statistics. More specifically, we calculate size and disorder dependencies of the relative fluctuation of

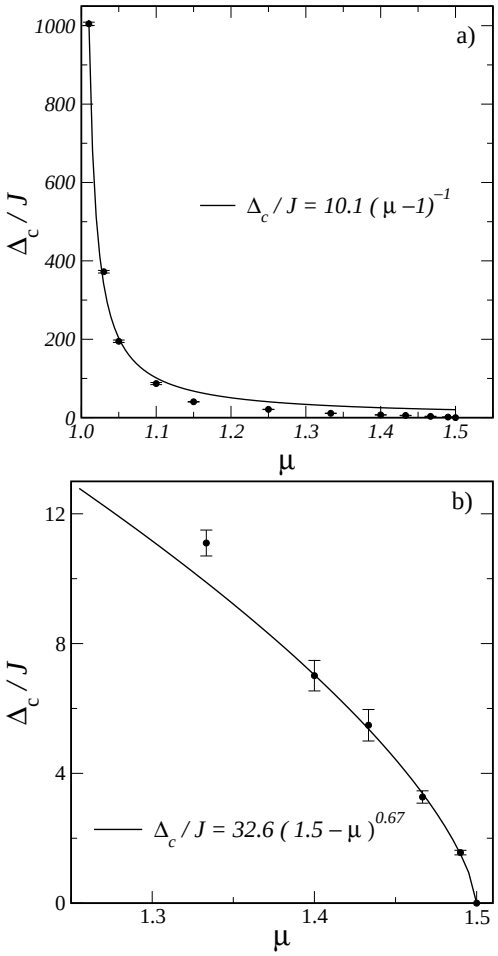

FIG. 1: Critical magnitude of disorder Δ_c as a function of the interaction exponent μ. Full circles represent the numerical data, while solid lines are the best fits: (a) $\mu \to 1$ and (b) $\mu \to 3/2$.

the participation number (PN) defined as

$$P_k = \left(\sum_{n=1}^{N} |\psi_{kn}|^4 \right)^{-1} \ , \tag{8}$$

where ψ_{kn} denotes the n-th component of the normalized k-th eigenstate of the Hamiltonian (1). Here, the state index k ranges from 1 to N. By definition, we adscribe band-edge states $k = 1$ and $k = N$ to the uppermost and lowermost eigenstates, respectively. It was demonstrated recently[37,38] that within the considered model, the ratio of the standard deviation of the PN (SDPN) to the mean of the PN (MPN) is an invariant parameter at transition and therefore can be used to detect the critical point. We note that wave function statistics turned out to be more efficient for this purpose than level statistics (the latter also represents a method to monitor the transition[34]), because wave function statistics appeared to be less affected by strong finite size effects within the model (for details see the discussion in Refs. 37-38).

As the LDT occurs at the top of the band within the considered model, we calculated disorder and size dependencies of the ratio SDPN/MPN for the uppermost state. Open chains were used in all calculations. Following the procedure developed in Ref. 38, we obtained the critical magnitude of disorder Δ_c at which uppermost eigenstates undergo the LDT for $\mu \in (1, 3/2]$. The results of the simulations are shown in Fig. 1 by the full circles, while solid lines represent best fits close to the limiting points $\mu = 1$ (Fig. 1*a*) and $\mu = 3/2$ (Fig. 1*b*). We found that

$$\Delta_c \approx 10.1J(\mu - 1)^{-1} , \qquad \mu \to 1 , \qquad (9a)$$

$$\Delta_c \approx 32.6J\,(3/2 - \mu)^{0.67} . \qquad \mu \to 3/2 , \qquad (9b)$$

First of all, we notice that, according to Eq. (9a), the critical magnitude of disorder diverges as $\Delta_c \propto (\mu-1)^{-1}$ when $\mu \to 1$. The explanation of the divergence relies in the fact that $\Delta_c \propto E_\mu^{\rm top}$ for $\Delta_c \gg 1$,[38] and the upper band-edge energy $E_{\mu=1}^{\rm top}$ diverges when $N \to \infty$ as $(\mu - 1)^{-1}$. Contrary to that, the critical magnitude of disorder vanishes as $\Delta_c \propto (3/2 - \mu)^{0.67}$ when $\mu \to 3/2$, indicating that in the marginal case ($\mu = 3/2$) the uppermost state is localized ($\Delta_c = 0$), in full agreement with the results obtained by the renormalization group approach combined with a super-symmetric method for disorder averaging.[41]

IV. MOBILITY EDGE AND FRACTION OF THE DELOCALIZED STATES

Having discussed the dependence of the critical magnitude of disorder Δ_c on the interaction exponent μ for the uppermost state, we now focus on the mobility edge and the fraction of extended states in the thermodynamic limit. This question has not been addressed in previous studies,[37,38,39,40,41,42] except for a comment on the existence of a single mobility edge[40,41] (see also the discussion in Sec. II).

To work out this problem, we numerically diagonalized the Hamiltonian (1) and calculated the normalized MPN, $\langle P\rangle/N$, as a function of energy for different system sizes N. The results of these simulations are shown in Fig. 2 for a particular set of interaction exponent and magnitude of disorder ($\mu = 5/4$ and $\Delta = 5J$). First, one can see that the upper band-edge energy increases with N as was mentioned in Sec. III (see also Refs. 37-38). Note also the noticeable size dependence of the normalized MPN of the uppermost state. This behavior reflects the finite size effects already mentioned above (see the preceding section). The boundaries result in a positive correction of the order of $N^{-\mu}$ to the *bulk* value of the uppermost wave function ($\sim 1/\sqrt{N}$). Consequently, the normalized MPN depends on the system size as $(1 - c\,N^{1-\mu})$, where c is a constant. The second, and the most important, observation is that the normalized MPN increases monotonically on approaching the upper band edge, for all considered values of N.

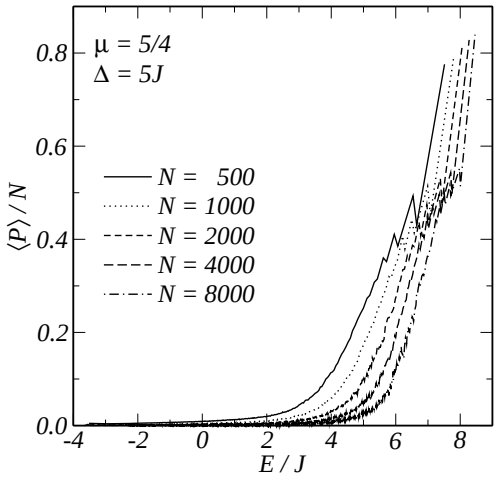

FIG. 2: The normalized mean participation number $\langle P_k\rangle/N$ as a function of energy for different system sizes N calculated for the interaction exponent $\mu = 5/4$ and the disorder strength $\Delta = 5J$.

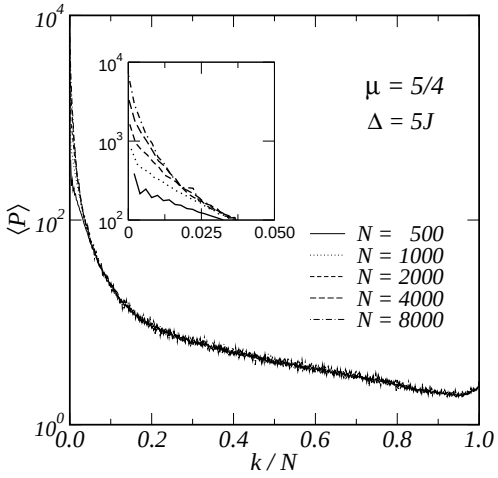

FIG. 3: The mean participation number as a function of the normalized state index k for different system sizes N calculated for the interaction exponent $\mu = 5/4$ and the disorder strength $\Delta = 5J$. The inset shows an enlarged view close to the upper band edge.

In order to avoid the size dependence of the upper band-edge, we use hereafter the state index k rather than the energy $E_\mu(k)$. In Fig. 3 we plotted the MPN as a function of the normalized state index k/N. The figure demonstrates that the MPN is independent of the system size in a wide range of the normalized state index k/N. The perfect collapse of the curves within this range clearly indicates the localized nature of these eigenstates. However, at the top of the band the MPN increases linearly with the system size and the collapse is absent (see the blow-up in the inset of Fig. 3). This result suggests that not only the uppermost eigenstate, but a number of them are delocalized, in agreement with the previous claim raised in Ref. 41

We now apply a finite size analysis of our numerical results to further confirm the latter statement and to obtain the size scaling of the number of extended eigenstates. Figure 4 shows that the MPN for different sizes collapses onto a single curve close to the top of the band after introducing the rescaled index $k/N^{1/3}$ for $\mu = 5/4$. The collapse holds up to a finite value of the rescaled index, which indicates that the number of extended states scales as $\propto N^{1/3}$ when $\mu = 5/4$.

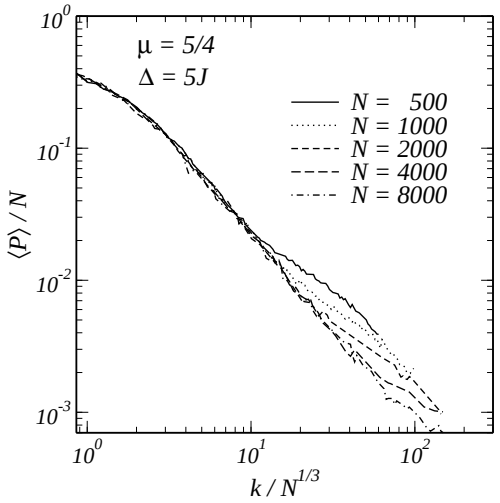

FIG. 4: Normalized mean participation number as a function of $k/N^{1/3}$ for different system sizes calculated for $\mu = 5/4$ and $\Delta = 5J$.

To provide support to these numerical results, we now develop a simple (perturbative) analytical approach that allows us to understand the origin of the obtained results. To this end, we analyze the energy spacing close to the upper band-edge in the disorder-free system ($\Delta = 0$) more accurately. The spacing can be obtained from Eq. (3):

$$\delta E_\mu^{\rm top}(k) = J\, C_\mu\, \frac{1}{k}\left(\frac{k}{N}\right)^{\mu-1} . \qquad (10)$$

The constant C_μ absorbs all unessential numerical factors. Note the absence of the scaling of the spacing $\delta E_\mu^{\rm top}(k)$, i.e., the spacing depends on k not only on k/N. This is crucial for the peculiar features of the LDT within the model. Indeed, consider a chain of a particular size N. Assume that the disorder is perturbative for the uppermost state ($k = 1$), i.e., $\sigma \ll \delta E_\mu^{\rm top}(1)$, so that states at the top are extended over the whole sample. Let us now find the *mobility edge* for this finite lattice, defining it by the equality

$$\delta E_\mu^{\rm top}(k_m) = \sigma . \qquad (11)$$

The number k_m, which is N-dependent, divides all eigenstates into two sets: those with $k < k_m$ are delocalized in the above sense, while eigenstates with $k > k_m$ are localized in the usual sense. Thus, k_m provides us with the number of extended states for a particular system size N. Determined by the equation (11) it reads

$$k_m = D_\mu \left(\frac{J}{\Delta}\right)^{1/(2-\mu)} N^{(3/2-\mu)/(2-\mu)} , \qquad (12)$$

where all unessential constants are absorbed into D_μ. Applying Eq. (12) to the particular case $\mu = 5/4$ we recover the behavior that we have found numerically, namely $k_m \propto N^{1/3}$.

The relationship (12) provides us also with the dependence of k_m on the disorder magnitude Δ, which can also be compared to numerical calculations. We performed such comparison for the interaction exponent $\mu = 5/4$. In this particular case, the exponent $1/(2-\mu)$ in the Δ-dependence of k_m is equal to 4/3. Figure 5 shows the normalized mean participation number as a function of $k\Delta^{4/3}$ calculated for different disorder strength Δ and a given system size $N = 4000$. The collapse of all curves onto a single one in the vicinity of the upper band-edge supports the validity of Eq. (12).

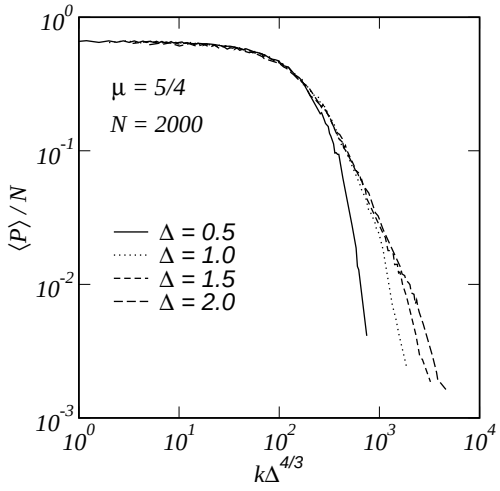

FIG. 5: Normalized mean participation number as a function of $k\Delta^{4/3}$ for different disorder magnitudes with $\mu = 5/4$ and $N = 2000$.

We have also tested Eq. (12) against numerical simulations performed for other values of $\mu \in (1, 3/2)$ and always found an excellent agreement of the numerical data with the analytic formula (12). It follows from the formula that the number of extended states increases sublinearly with the system size, namely as $N^{(3/2-\mu)/(2-\mu)}$, which means that the fraction of these states vanishes as $N^{-1/(4-2\mu)}$ when $N \to \infty$. From this we conclude that the mobility edge approaches to the upper band edge in the thermodynamic limit.

V. SUMMARY AND CONCLUDING REMARKS

We studied both analytically and numerically the localization properties of the 1D tight-binding model with

diagonal disorder and *non-random* long-range inter-site interactions, $J_{mn} = J/|m-n|^{\mu}$ where $J > 0$. The model can be critical at the upper band-edge provided $1 < \mu < 3/2$.

We calculated the phase diagram of the transition (the dependence of the critical magnitude of disorder Δ_c on the interaction exponent μ) by studying the participation number statistics. The critical magnitude of disorder was detected using the size invariance of the ratio of the standard deviation to the mean. We found that Δ_c diverges as $(\mu-1)^{-1}$ when $\mu \to 1$, which originates from the similar divergence of the upper band-edge energy. If $\mu \to 3/2$, the critical disorder magnitude vanishes as $(3/2-\mu)^{2/3}$, indicating that all states are localized at $\mu = 3/2$, no matter how small the disorder is.

It is shown, both analytically and by means of the finite size scaling analysis, that the number of extended states at the upper band-edge increases sub-linearly with the system size N, namely as $\propto N^{(3/2-\mu)/(2-\mu)}$), therefore forming a set of null measure in the density of states in the thermodynamic limit. This suggests that the mobility edge is only a meaningful concept for a finite size system; it approaches to the upper band-edge in the thermodynamic limit. Although extended states form an infinitesimal fraction of the whole density of states, they can provide a strong impact on the transport properties, similarly to what happens in systems with correlated randomness.[11,12,15]

To conclude, we note that our findings, apart from being interesting from the theoretical point of view, are relevant for real physical systems. Thus, some organic materials with planar geometry, in which optically allowed excitations are dipolar Frenkel excitons,[45,46,47,48,49,50,51,52] represent an example; the value of the interaction exponent for the dipole-dipole inter-site interaction is $\mu = 3$, which resembles the weak localization regime in the 1D long-range model when $\mu = 3/2$.[41] Dipole-exchange spin waves in ferromagnetic films provide yet another example where these results are relevant.[53]

Acknowledgments

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